Sarcosine, N-(2-thienylcarbonyl)-, butyl ester

Inchi: InChI=1S/C12H17NO3S/c1-3-4-7-16-11(14)9-13(2)12(15)10-6-5-8-17-10/h5-6,8H,3-4,7,9
InchiKey: NAIBAEQJVQOMBR-UHFFFAOYSA-N
Formula: C12H17NO3S
SMILES: CCCCOC(=O)CN(C)C(=O)c1cccs1
Mol. weight [g/mol]: 255.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	2.163		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321464&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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